UCRL-CONF-208593

LAWRENCE
LIVERMORE
NATIONAL
LABORATORY

Advantages of Analytical Transformations in Monte Carlo Methods for Radiation Transport

M. S. McKinley, E. D. Brooks III, F. Daffin

December 14, 2004

The Monte Carlo Method: Versatility Unbounded In A Dynamic Computing World
Chattanooga, TN, United States
April 17, 2005 through April 21, 2005

The Monte Carlo Method: Versatility Unbounded In A Dynamic Computing World
Chattanooga, Tennessee, April 17–21, 2005, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2005)

Advantages of Analytical Transformations in Monte Carlo Methods for Radiation Transport

Michael Scott McKinley, Eugene D. Brooks III and Frank Daffin
Lawrence Livermore National Laboratory
7000 East Ave., Livermore, CA 94551
mckinley9@llnl.gov; brooks3@llnl.gov; daffin1@llnl.gov

ABSTRACT

Monte Carlo methods for radiation transport typically attempt to solve an integral by directly sampling analog or weighted particles, which are treated as physical entities. Improvements to the methods involve better sampling, probability games or physical intuition about the problem. We show that significant improvements can be achieved by recasting the equations with an analytical transform to solve for new, non-physical entities or fields. This paper looks at one such transform, the difference formulation for thermal photon transport, showing a significant advantage for Monte Carlo solution of the equations for time dependent transport. Other related areas are discussed that may also realize significant benefits from similar analytical transformations.

Key Words: Difference formulation, radiation transport

1 INTRODUCTION

In radiation transport, Monte Carlo methods offer several advantages such as parallelism and arbitrary geometry. However, Monte Carlo methods in thermal photon transport do have a couple of obstacles to overcome. The first is the stiff coupling between the radiation and the material in thick media. The second is that in thick systems, noise in the solution is quite high and it takes a quadratic amount of computer time to drive this noise down.

For a thick system, the system tends “locally” to the “local steady-state solution.” It does not make much sense to spend a lot of computer time solving a known solution. This is the idea behind the *difference formulation* [1]. For thermal photons, the steady-state solution is the black-body field for the local temperature. There is little to be gained from computing this known analytical solution. So instead of solving for the local radiation field, one can solve for the difference between the radiation field and the steady-state solution. As the system approaches steady-state, the difference field would shrink as well as the noise. This has been demonstrated in local thermodynamic equilibrium [2] and line transport [3].

Section 2 will give an overview of solving an analytical transformation with the example being photon transport in local thermodynamic equilibrium (LTE). Section 3 shows the standard formulation in one dimension in the LTE regime while Section 4 shows the difference formulation analytical transform. Section 5 shows some computational results that demonstrate the savings of using this transform. We conclude in Section 6 with the advantages of using transforms and other areas of possible interest.

2 ANALYTICAL TRANSFORM EXAMPLE

This paper demonstrates an analytical transform example using photon transport in LTE. Interest in this field initially sparked the desire to find ways of making photon transport in Monte

Carlo run faster. Transporting through thick materials, such as in stellar atmospheres, leads to very noisy answers. Implicit (effective) scattering is also responsible for consuming computer time.

Implicit solutions were first used to solve this radiation transport problem back in 1971 [4]. Implicit values are the end of the time step values used in evaluating quantities during the time step, while explicit values are the initial values at the beginning of the time step. Explicit Monte Carlo of the radiation was found to be unstable, and so a partially implicit solution was invented by Fleck. However, as part of the solution, some of the absorption was changed into an effective scattering cross section that was dependent on the time step size and optical thickness. So while it gained stability, it also led to an increase in scattering events which required more computer time.

A further step in reducing the computer time was the Symbolic Implicit Monte Carlo Method (SIMC) [5, 6]. SIMC is an expected value approach where particle weight is treated symbolically and attenuated as it travels through a medium. This had the benefit of getting rid of the effective scattering term. The downside is that SIMC requires a nonlinear system solve at the end of each time step.

A new attempt was made to formulate the problem with a different approach. The idea was based on the observation that in thick media, the standard formulation was leading towards a subtraction of two large numbers, emission and absorption, of which one was determined by Monte Carlo sampling. In addition, an analytical answer was known for steady-state, so a lot of computation was being wasted with a solution that was not far from steady-state.

So the transport equations were transformed as detailed in Section 4 to give a new set of equations for which the difference field is the quantity of interest. Therefore, the field is expected to be close to zero. The Monte Carlo noise is also expected to be low as well since our solution is expected to be small. In addition, we can shuffle particles to put more particles in regions of change where better statistics are needed to get the solution. In Section 5, we show some results from a test run that vindicate this line of reasoning.

The biggest lesson learned is that one should look at common problems and see where the computational time is being spent. If it is being spent computing something known, then a recasting of the equations with an analytical transform may be of some benefit. The new equations may mathematically indicate transport of some odd quantity. In the example presented in this paper, negative weights are transported. However, it all works out if one visualizes negatively weighted particles as being “missing particles” relative to the background radiation field. Similar transformations are used in semiconductors, where electrons and holes are the transported quantities. Other transformations may be possible for the different types of solutions envisioned. In addition to LTE, the difference formulation has also been applied to line transport [3].

3 LTE STANDARD FORMULATION

The standard formulation of the transport equation in LTE, without scattering in slab geometry is given as

$$\frac{\partial I(x,t,\nu,\mu)}{\partial t} + \mu c \frac{\partial I(x,t,\nu,\mu)}{\partial x} = \\ - c\sigma_a^{'}(\nu, T(x,t))[I(x,t,\nu,\mu) - B(\nu, T(x,t))] \tag{1}$$

$$\frac{\partial E_{mat}}{\partial t} = \int_0^\infty d\nu \int_{-1}^1 d\mu \sigma_a^{'} [I(x,t,\nu,\mu) - B(\nu, T(x,t))] + G \tag{2}$$

where I is the specific intensity of the photons, t is time, μ is the cosine of the angle of the particle with respect to the x-axis, x is position, ν is the photon frequency, c is the speed of light, $\sigma_a^{'}$ is the absorption cross section, B is the thermal (Planck) distribution at the material temperature (T), E_{mat} is the material energy density and G is any external volumetric energy source. The blackbody function is defined as

$$B(\nu, T) = \frac{2h\nu^3}{c^2}\left(e^{h\nu/kT} - 1\right)^{-1} \tag{3}$$

where h is the Plank constant and k is the Boltzmann constant. We can express the blackbody function in terms of a "reduced" frequency distribution function as follows:

$$B(\nu, T) = \frac{caT^4}{4\pi} b(\nu, T) \tag{4}$$

$$\int_0^\infty d\nu b(\nu, T) = 1 \tag{5}$$

where a is the radiation constant. Equation (5) shows that b is normalized and this function is used to sample the frequency.

The final piece of the problem is the relationship between the material energy and the material temperature. The following relationship is used:

$$dE_{mat} = \rho c_v dT \tag{6}$$

where ρ is the density and c_v is the specific heat.

Showing the solution to all of this is beyond the scope of this paper. Instead a summary of the resulting procedure will be presented. We begin the Monte Carlo algorithm by sampling particles from Eq. (1) by using $\sigma_a^{'} B$ as the source and $\sigma_a^{'}$ as the loss coefficient. In this piecewise constant approach where all values are assumed to have a single value within a spatial zone, particles are emitted uniformly in time, space and angle within a spatial zone. Frequency is sampled from the "reduced" Plankian, *b*. In our discretization, the weight of each energy density particle is given as

$$W = c\Delta t \Delta x \sigma_a^{'} a T^4 \tag{7}$$

where Δt is the time step and Δx is the zone width. The T^4 factor is treated implicitly by marking the particle as "symbolic" and transporting the particle normally. However, the symbolic particles are scored differently because they are indexed by the zone in which they were born.

Once particle tracking is finished, I as a function of T^4 is placed in Eq. (2). This turns Eq. (2) along with Eq. (6) into a set of nonlinear equations with zone temperature as the unknown. One can solve this with a nonlinear system to arrive at new temperatures. Then all symbolic particles can be turned into regular numerical particles since the unknown T^4 of their birth zone is now known.

4 LTE DIFFERENCE FORMULATION

The difference formulation for LTE is a simple analytical transformation. It was noticed that at steady-state or in thick systems, the difference, $I - B$, is close to 0 and has a lot of Monte Carlo noise. In order to take advantage of this, a new variable was introduced, $D = I - B$. This changes Eqs. (1) and (2) to the following:

$$\begin{aligned} \frac{\partial D(x,t,\nu,\mu)}{\partial t} + \mu c \frac{\partial D(x,t,\nu,\mu)}{\partial x} &= -c\sigma_a^{'}(\nu, T(x,t)) D(x,t,\nu,\mu) \\ &\quad - \frac{\partial B(\nu, T(x,t))}{\partial t} - \mu c \frac{\partial B(\nu, T(x,t))}{\partial x} \end{aligned} \tag{8}$$

$$\frac{\partial E_{mat}}{\partial t} = \int_0^\infty d\nu \int_{-1}^1 d\mu \sigma_a^{'} D(x,t,\nu,\mu) + G \tag{9}$$

These two equations are very similar to the standard formulation equations. Both the difference formulation and the standard formulation have the same loss coefficient, $\sigma_a^{'}$. However, their biggest difference is in the source terms. The new source terms are $-\partial B / \partial t$ and $-\mu c \partial B / \partial x$. These source terms are quite different from the standard source because of the different particle distribution and possible negatively weighted.

4.1 Temporal Source Term

The $-\partial B / \partial t$ term produces particles of energy with weight as follows:

$$W_{\partial B / \partial t} = -\frac{a}{2\pi} \Delta x \left(T_{t_0 + \Delta t}^4 - T_{t_0}^4 \right) \tag{10}$$

where the temperatures are evaluated for each zone at the beginning and end of the time step. In this case the weight is made up of both explicit ($T_{t_0}^4$) and implicit ($T_{t_0+\Delta t}^4$) terms. The particles are emitted uniformly in time, space and angle just as in the standard formulation. However, the frequency distribution is quite different. The probability distribution function for the frequency is given as

$$pdf = \frac{b(\nu,\mathrm{T}_1)T_1^4 - b(\nu,\mathrm{T}_2)T_2^4}{T_1^4 - T_2^4} \tag{11}$$

where T_1 and T_2 represent the initial and final temperatures. There are two extremes to this distribution function. The first is when one temperature is zero. In that case, the frequency is sampled from the "reduced" Plankian. The other extreme case is when the temperatures are close to being equal. When this happens, the probability distribution function is

$$\lim_{T_1 \to T_2} \frac{b(\nu,\mathrm{T}_1)T_1^4 - b(\nu,\mathrm{T}_2)T_2^4}{T_1^4 - T_2^4} = \frac{4\pi}{ca}\frac{dB(\nu,T)}{dT^4}. \tag{12}$$

All other sampling is done directly from Eq. (11).

4.2 Spatial Source Term

The spatial term, $-\mu c\partial B/\partial x$, is much like the temporal term except for a few key differences. The weight of these energy particles are given as

$$W_{\partial B/\partial x} = -\frac{ca\Delta t}{8\pi}\left(T_i^4 - T_{i-1}^4\right) \tag{13}$$

where the index, i, is the index of a zone. Unlike all other source particles mentioned, emission occurs only on zone boundaries since temperature values are computed as piecewise constant within a zone and the derivative of a step function is a delta function. Emission is uniform in time. Like the previous temporal source particles, these particles are emitted with the same probability distribution as given by Eq. (11), except T_1 and T_2 are the temperatures on either side of a boundary.

The other difference in emission is in the angle. The probability distribution function is 2μ. Integration of this from -1 to 1 yields zero and leads to a problem of determining the angle of emission. However, insight to the problem shows that this can be represented as a pair production of particles. One with weight, W, in the forward direction and another with weight, -W, in the opposite direction. Now the integration is from 0 to 1 and the emission is forward peaked. This represents the flow of energy across a zone where negative weight is transporting the missing particles from the background radiation leaking from that zone.

5 COMPUTATIONAL RESULTS

A sample text problem is used to show the biggest advantage in this analytical transform. This problem is a 10 cm slab which is heated on the left and exposed to a vacuum on the right. The slab is made of a single material with a frequency independent (grey) opacity and a constant specific heat, 0.1 jerk/(keV cm^3), where a jerk is 10^{16} ergs. The initial temperature of the slab is 0.01 keV and the radiation is at equilibrium with the temperature. At time, $t = 0$, we turn on the 1 keV heat source on the left.

The problem is run with time steps of 0.2 shakes, where a shake (sh) is 10^{-8} seconds. The opacity is varied to be 1, 10, 100 and 1000 optical depths and the final time of the run is 20 sh, 20 sh, 40 sh and 320 sh, respectively. The problem is run until it is in an interesting enough state so that heat has transferred and is approaching steady-state.

The difference formulation and the standard formulation are compared using SIMC method. Since the goal is to compare the Monte Carlo and not the nonlinear system solve, the number of particles is dialed so that the nonlinear system solve is a small part of the computational time. The number of particles in the difference formulation is arbitrarily set to be 1/3 from the temporal source and 2/3 from the spatial source.

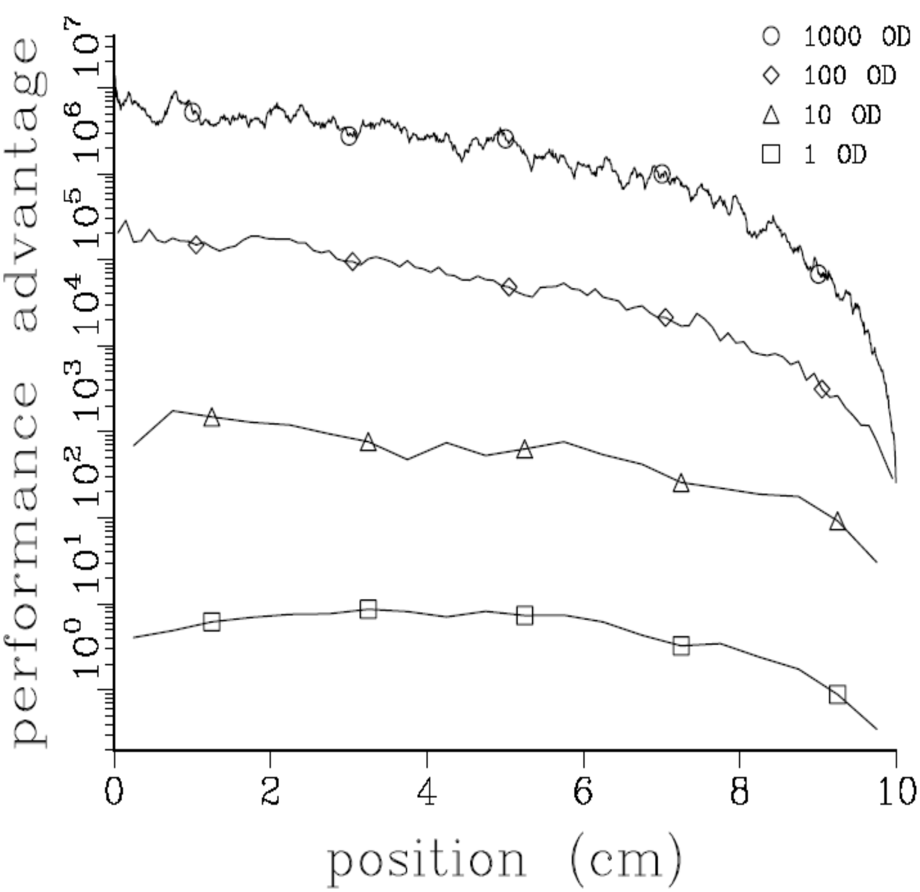

Figure 1. Performance advantage across the slab for each opacity as a function of position within the slab.

Figure 1 shows the ratios of the variances of the temperature of the slab calculated using the standard formulation to that calculated using the difference formulation. This figure shows the computational advantage for each position in the slab. In the case of 1 optical depth, the difference formulation is about 10 times better in some spots and falls to be worse than the standard formulation at the far right. On the whole, little is gained by using the difference formulation for this thin problem.

However, when the optical depth is increased to 10, the performance starts to skyrocket. While it follows the same trend as before, the average computational advantage has risen to 100. In other words, the standard formulation would have to be run 100 times longer to get the same reduction in Monte Carlo noise as the difference formulation.

Going to 100 and 1000 optical depths reveals an average computational advantage of 10,000 and 1,000,000, respectively. In this regime, the difference formulation has a huge savings because there is little work being done computing the temperatures of zones that are barely changing over time. In thick problems, the performance advantage can be leveled off by preferentially placing more particles in the underperforming zones.

6 SUMMARY & CONCLUSIONS

The difference formulation has been shown to be a powerful analytical transformation of the standard transport equation for photon transport. In high opacity regions when the Monte Carlo transport dominates, a high computational advantage can be expected. Since the difference formulation is transporting the difference field, the Monte Carlo noise is high in regions of temperature change such as the boundary or along a wave front.

The difference formulation has areas of optimization that we have not studied. While it is obvious that particles need to be placed preferentially in areas of change, detecting these areas requires some work. Difference particles can be from the spatial term or the temporal term. However, the optimal ratio of emission of each type of source particle is not well understood. Each type of particle seeks to bring balance to the transport equation by monitoring heat flow over time as well as over space. So deciding which is most important during a problem is a further area of improvement.

In the difference formulation, emission does not require sampling a frequency dependent opacity that depends upon complex material properties as is done in the standard formulation. Therefore, sampling the emission profile in the difference formulation is simpler since emission is not material dependent. Sampling the frequency in difference formulation has been worked out as a simple set of algorithms [2].

Future work in the difference formulation involves looking at linear values as opposed to piecewise constant values over a zone. This should smooth out some problems with energy "teleporting" across a zone. This "teleporting" occurs when absorption of a photon entering the zone at the end of one time step may be emitted at the other end of the zone at the beginning of the next time step. Thus energy may seem to transport faster than the speed of light in the material.

Another possible direction for future work lies in looking at the difference formulation for deterministic methods. Since the difference formulation is based in the numerical trick for removing the subtraction of large numbers, this same trick may have benefits in some deterministic methods as well.

One last area of future work is in looking at non-analytical transforms. An example of this could be solving for the neutron flux across a reactor using a quick method such as diffusion or guessing at the flux shape. Instead of transporting neutrons, transport the difference of the neutron flux and the flux as determined by the quick method. This may lead towards savings in Monte Carlo noise in certain cases. For example, ongoing work in residual, implicit Monte Carlo methods for nonlinear, discrete radiation transport demonstrates the gains possible from a Monte Carlo transformation. [7-13]

7 ACKNOWLEDGMENTS

This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

8 REFERENCES

1. A. Szoke, E. D. Brooks III, "The Transport Equation in Optically Thick Media," *J. Quant. Spectr. Rad. Transfer*, **91**, pp.95-110 (2005).
2. E. D. Brooks III, M. S. Mckinley, F. Daffin, A. Szoke, "Symbolic Implicit Monte Carlo Radiation Transport in the Difference Formulation: A Piecewise Constant Discretization," *submitted to Journal of Computational Physics* (2005).
3. F. Daffin, M. S. McKinley, E. D. Brooks III, A. Szoke, "An Evaluation of the Difference Formulation for Photon Transport in a Two Level System," *submitted to Journal of Computational Physics* (2005).
4. J. A. Fleck, Jr., J. D. Cummings, "An Implicit Monte Carlo Scheme for Calculating Time and Frequency Dependent Radiation Transport," *J. Comput. Phys.*, **8**, pp.313-342 (1971).
5. E. D. Brooks III, "Symbolic Implicit Monte Carlo," *J. Comput. Phys.*, **82**, pp.433-446 (1986).
6. T. N'kaoua, "Solution of the Nonlinear Radiative Transfer Equation by a Fully Implicit Matrix Monte Carlo Method Coupled with the Rosseland Diffusion Equation via Domain Decomposition," *SIAM J. Sci. Stat. Comput.*, **12**, pp.505-520 (1991).
7. J. Halton, "Sequential Monte Carlo Techniques for the Solution of Linear Systems," *J. Sci. Comput.*, **9**, pp. 213-257 (1994).
8. T. Booth, "Exponential Convergence on a Continuous Monte Carlo Transport Problem, *Nucl. Sci. Eng.*, **127**, pp. 338-345 (1997).
9. J. Favorite, H. Lichtenstein, "Exponential Monte Carlo Convergence of a Three-Dimensional Discrete Ordinates Solution, *Trans. Am. Nucl. Soc.*, **81**, pp 147-148(1999) 147–148.

10. H. Lichtenstein, “Exponential Convergence Rates for Reduced-Source Monte Carlo Transport in [x,μ] Geometry,” *Nucl. Sci. Eng.*, **133**, pp. 258-268 (1999).
11. T. Booth, “Adaptive Importance Sampling with a Rapidly Varying Importance Function,” *Nucl. Sci. Eng.*, **136**, pp 399-408 (2000).
12. T. Booth, “An Approximate Monte Carlo Adaptive Importance Sampling Method,” *Nucl. Sci. Eng.*, **138**, pp. 96-103 (2001).
13. T.M. Evans, et. al. “A Residual Monte Carlo Method for Discrete Thermal Radiative Diffusion,” *J. Comput. Phys.*, **189** pp. 539–556 (2003).